HIGH RESOLUTION ELECTRONIC SPECTROSCOPY OF PHENOL-METHANOL

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The rotationally resolved electronic spectrum of the hydrogen bonded phenol(MeOH)₁ cluster at 35933 cm⁻¹ in a molecular beam is presented. The vibronic origin band consists of two sub-spectra separated by approximately 3.5 GHz, exhibiting an intensity ratio of approximately 16:9, with the weaker band shifted to higher frequencies. Both sub-spectra are *ab* hybrid bands with an intensity ratio of $I_a/I_b = 1/3$.

As in phenol $(H_2O)_1^a$ the phenolic moiety acts as proton donor in this cluster system. The observed splitting into sub-bands is attributed to the methyl group internal rotation, however. This differs from phenol $(H_2O)_1$ that shows a splitting due to a torsional motion of water. From the obtained data we determine parameters of the intermolecular structure of the cluster as well as for the torsional potential of the methyl rotation.

^aG. Berden, W.L. Meerts, M. Schmitt and K. Kleinermanns, J. Chem. Phys. 104 (1996), 972.